

# The underscreened Kondo effect: a two S=1 impurity model

Karyn Le Hur and B. Coqblin

*Laboratoire de Physique des Solides, Université Paris-Sud, Bât. 510, 91405 Orsay, France*

## Abstract

The underscreened Kondo effect is studied within a model of two impurities S=1 interacting with the conduction band and via an interimpurity coupling  $K\vec{S}_1.\vec{S}_2$ . Using a mean-field treatment of the bosonized Hamiltonian, we show that there is no phase transition, but a continuous cross-over versus K from a non Kondo behaviour to an underscreened Kondo one. For a small antiferromagnetic coupling ( $K_I < 0$ ), a completely asymmetric situation is obtained with one  $s=\frac{1}{2}$  component strongly screened by the Kondo effect and the other one almost free to yield indirect magnetism, which shows finally a possible coexistence between a RKKY interaction and a local Kondo effect, as observed in Uranium compounds such as  $UPt_3$ .

**PACS.** numbers: 75.20.Hr, 75.30. Mb, 71.27. +a

## I. INTRODUCTION

Kondo Cerium compounds have been extensively studied from both experimental and theoretical point of view. In this case, the Kondo effect is well described by either the s-f exchange Hamiltonian with a  $S^f = \frac{1}{2}$  spin screened by only one conduction electron channel [1] or the so-called Coqblin-Schrieffer Hamiltonian [2] when orbital degeneracy and spin-orbit coupling are taken into account; in the two preceding cases, there is an equal number of 4f and conduction electrons. The ground state of the regular Kondo effect is a nonmagnetic singlet state in the case of a single impurity [1] and the low temperature properties are characterized by a Fermi-liquid behaviour. In the case of heavy-fermion compounds, there is a strong competition between the Kondo effect and the magnetic ordering, which yields either nonmagnetic or magnetically ordered Cerium Kondo compounds [3,4].

On the other hand, some Uranium compounds, such as  $UPt_3$ , present also a heavy-fermion behaviour and are also superconducting.  $UPt_3$  has an outstanding behaviour, since it undergoes a transition to an antiferromagnetic ordering with a tiny ordered magnetic moment of  $0.02 \pm 0.01 \mu_B$  below a Neel Temperature  $T_N \sim 5K$  [5] and becomes superconducting below  $T_c \sim 0.5K$  [6]. A heavy-fermion behaviour characterized by a large electronic specific heat constant  $\gamma \sim 0.4 \text{ J/moleK}^2$  [7] and a  $T^2$  term of the resistivity [8] is observed in  $UPt_3$  at low temperatures. A third characteristic temperature  $T_S = 17.6K$  given by the maximum of the magnetic susceptibility corresponds approximatively to the onset of spin fluctuations [8]. The heavy-fermion character decreases with pressure [7,8], while the antiferromagnetic order disappears at roughly 5 kbar [9].

The real nature of the magnetic order in  $UPt_3$  is still a controversial subject, because no small-moment antiferromagnetism has been observed in a recent  $\mu$ SR study of pure  $UPt_3$  [10]. Neutron-diffraction experiments [11] have been also recently carried out on single-cristalline samples of the heavy-fermion pseudobinary alloys  $U(Pt_{1-x}Pd_x)_3$ . At low Pd concentrations,  $x=0.002$  and  $x=0.005$ , small-moment magnetic order is observed below 6K, just like in  $UPt_3$ . For large  $x$  values, a clear magnetic order exists, with a magnetic moment

of  $0.35 \mu_B$  for  $x=0.02$  and  $0.62 \mu_B$  for  $x=0.05$  and with an increasing Neel Temperature  $T_N=3.5\text{K}$  for  $x=0.02$  and  $T_N=5.9\text{K}$  for  $x=0.05$ . These recent experiments on  $UPt_3$ -based alloys show that the magnetic order is a regular antiferromagnetic one for  $x \geq 0.02$ , while the origin of the magnetic order is still controversial for  $UPt_3$ ; the question arises to know if the magnetic moment of  $UPt_3$  is a real long-range one or a so-called "short-range" with a very large correlation length.

Other Uranium compounds namely  $UBe_{13}$  [12],  $URu_2Si_2$  [13],  $UNi_2Al_3$  [14–16] and  $UPd_2Al_3$  [14–16] present also at low temperatures a weak magnetic ordering with small magnetic moments, followed at still lower temperatures by a transition to a superconducting state. These Uranium compounds are characterized by a Neel temperature ( $T_N=8.8\text{K}$  in  $UBe_{13}$  [17],  $17.5\text{K}$  in  $URu_2Si_2$  [13],  $4.6\text{K}$  in  $UNi_2Al_3$  [16] and  $14\text{K}$  in  $UPd_2Al_3$  [16]) larger than the superconducting temperature (respectively  $0.85\text{K}$ ,  $0.8\text{K}$ ,  $1\text{K}$  and  $2\text{K}$ ) and by large values of the electronic specific heat constant  $\gamma$ . The values of the magnetic moments are rather small, except in the case of  $UPd_2Al_3$  where an ordered magnetic moment of  $0.85 \mu_B$  has been deduced from an elastic neutron scattering study [18]. The origin of these small magnetic moments and the eventual similarity between Uranium and Cerium compounds as  $CeCu_2Si_2$  have been discussed in many papers [19–21]. The exact nature of the magnetic ordering in these Uranium compounds is not definitively established. However the existence of both a heavy-fermion character and a weak-magnetic ordering seems to be characteristic of Uranium compounds, while the question is more controversial in Cerium compounds such as  $CeCu_2Si_2$ , where the existence of a weak magnetic order has not been definitively established and any way depends on the sample composition [20]. According to Steglich et al, [20] recent experiments support the coexistence of two possible channels of so called "localized" and "itinerant" 5f states in Uranium compounds and these two 5f subsystems appear to be only weakly coupled to each other in  $UPd_2Al_3$  for example.

Thus, the purpose of the present paper is to present an explanation for the coexistence of the heavy-fermion character and tiny ordered magnetic moments in Uranium compounds such as  $UPt_3$ . This explanation is based on the "underscreened Kondo model" which appears

to be appropriate to describe the  $5f^2$  configuration of Uranium atoms.

The underscreened Kondo model corresponds to the case  $2S > n$ , where  $S$  is the localized spin and  $n$  the number of screening channels coming from conduction electrons [22]. We will describe here the simple case of the underscreened Kondo effect with  $S=1$ ,  $n=1$  but indeed it is certainly necessary to include the orbital degeneracy and spin-orbit effects to give a good description of compounds such as  $UPt_3$ .

The underscreened  $S=1$  one-impurity Kondo Hamiltonian is given by:

$$\mathcal{H} = \sum_{\vec{k}} \epsilon_{\vec{k}} \Psi_{\vec{k}}^\dagger \Psi_{\vec{k}} + J \sum_{\vec{k}, \vec{k}'} \Psi_{\vec{k}}^\dagger \vec{\sigma} \Psi_{\vec{k}'} \cdot \vec{S} \quad (1)$$

where  $\Psi_{\vec{k}}^\dagger = (\Psi_{\vec{k}, \uparrow}^\dagger, \Psi_{\vec{k}, \downarrow}^\dagger)$  is a conduction electron spinor and  $S$  is a  $SU(2)$  1-spin. The Hamiltonian (1) has been studied in the general context of the underscreened Kondo problem using renormalization methods [23] and has been solved exactly by the Bethe Ansatz [24] method and conformal theory arguments [25].

The ground state has a 2-fold degeneracy corresponding to an unquenched spin  $\frac{1}{2}$ , whose the residual coupling to the Fermi sea is ferromagnetic and scales to zero at low temperatures. The strong Fermi-liquid fixed point is **stable**. The low-energy electronic excitations are free-electron like and the many body interactions induced by the Kondo effect lead, at low energy, to a simple phase shift which is equal to  $\delta = \frac{\pi}{2}$ .

## II. GENERAL CONSIDERATIONS ON THE TWO-IMPURITY KONDO PROBLEM

The two-impurity Kondo problem with a spin  $s = \frac{1}{2}$  on each impurity, embedded in a conduction electron band with only one  $n=1$  channel, has been extensively studied by many authors in the last ten years. A recent review of the main works can be found in Ref. [26]. The two-impurity problem provides a simple model to study the competition between the Kondo effect and the indirect Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.

We would like to study here the two-impurity Kondo problem with a spin  $S=1$  on each

impurity and with only one  $n=1$  channel for conduction electrons. We consider two  $S=1$  spins symmetrically located about the origin and interacting with a Fermi gas. The total Hamiltonian is the sum of the three following terms:

$$\begin{aligned}
H_o &= \int d^3\vec{k} \ \epsilon(\vec{k}) \Psi_{\vec{k}}^{\alpha\dagger} \Psi_{\alpha\vec{k}} \\
H_k &= \int d^3\vec{k}_1 \int d^3\vec{k}_2 \ \Psi_{\vec{k}_1}^{\alpha\dagger} \sigma_{\alpha}^{\beta} \Psi_{\beta\vec{k}_2} \cdot [V(\vec{k}_1)^* V(\vec{k}_2) \vec{S}_1 + V(-\vec{k}_1)^* V(-\vec{k}_2) \vec{S}_2], \\
H_i &= K \vec{S}_1 \vec{S}_2
\end{aligned} \tag{2}$$

where  $S_1$  and  $S_2$  are two  $S=1$  impurities.  $V(\vec{k})$  is proportionnal to the Anderson model hybridization matrix element and we adopt here the particular choice of Ref. [26].  $V(\vec{k})$  and  $K$  are considered as two independent parameters. The parameter  $K$  takes into account both, all the direct exchanges between  $S_1$  and  $S_2$  and the RKKY interaction between two  $s=1/2$  spins (one of  $S_1$  and the second of  $S_2$ ), defined by:

$$K(R) = \frac{J^2 \cos 2k_F R}{E_F (2k_F R)^3} \tag{3}$$

where,  $R$  is the distance between  $S_1$  and  $S_2$  and  $E_F$  is the energy at the Fermi level.

There are two stable obvious limits for this problem:

- when  $K \longrightarrow +\infty$ , the two  $S=1$  spins tend to form a singlet of spin and, therefore, the electron gas is not affected by the presence of these two impurities. There are no Kondo effect and a zero phase shift  $\delta$  for the conduction band.
- when  $K \longrightarrow -\infty$ , on the contrary, the two impurities behave as an effective single  $S=2$  impurity with  $n=2$  channels of conduction electrons interacting with it. In this Kondo effect, only a  $S=1$  spin of the effective impurity is screened; the remaining low-energy conduction electron degrees of freedom are decoupled from it, but yield a  $\delta = \frac{\pi}{2}$  phase shift in both channels. It corresponds to a local Fermi-liquid-fixed-point and, therefore, the many-body interactions lead to a simple phase shift at low energy.

Thus, the purpose of the present paper is to study the  $S=1$  two-impurity problem for all  $K$  values. The central question is, therefore, to know if the local Fermi-liquid description

still holds for all  $K$  values at  $T=0$  or similarly if the phase shift of the conduction electrons varies continuously with  $K$  at  $T=0$ .

In the case of the two  $s = \frac{1}{2}$  Kondo impurities, there must be, as a function of  $K$ , a phase transition, but the existence of a critical point is still controversial, since for example numerical renormalization group calculations yield a critical point, while finite-temperature Monte Carlo (MC) calculations [27] do not show evidence for such a critical point. Thus, the question of an eventual phase transition has to be also discussed in our case of two  $S=1$  spins.

Thus, in the present section, we will present the main features of the two-impurity problem, which have been already developed for the  $s = \frac{1}{2}$  case, in particular in the recent papers of Affleck et al. [26] and Sire et al. [28]. The Hamiltonian (2) is transformed by using successively an one-dimension mapping and the classical bosonization technique, exactly as in the previous  $s = \frac{1}{2}$  case.

In the next section III, we will describe our work on the specific  $S=1$  two-impurity problem and we use successively the Jordan-Wigner transformation to refermionize the Hamiltonian and a specific mean field approximation to treat the problem. The different cases, especially  $K=0$  and  $K \neq 0$  for an antiferromagnetic coupling, will be then discussed.

### A. The one-dimensional mapping

We follow here the notations of the recent paper by Affleck et al [26] on the two  $s = \frac{1}{2}$  impurity case and we just recall the main points for our study of the two  $S=1$  impurities.

As usual, we consider a  $\delta$  function interaction in (2), with the impurities at  $\pm \frac{\bar{R}}{2}$ , so that:

$$V(\vec{k}) = V_o e^{i\vec{k} \frac{\bar{R}}{2}} \quad (4)$$

For certain choices for the dispersion relation  $\epsilon(\vec{k})$  and matrix element  $V(\vec{k})$ , the Hamiltonian (2) has a particle-hole (PH) symmetry. Invariance of  $H_o$  under the PH symmetry requires:  $\epsilon(\vec{k}) = -\epsilon(\vec{k}')$ , where  $\vec{k}$  and  $\vec{k}'$  are changed to each other by the PH symmetry.

Invariance of  $H_k$  under this PH symmetry requires:

$$V(\vec{k}') = V(\vec{k})^* \quad \text{and} \quad V(-\vec{k}') = V(-\vec{k})^* e^{i\eta} \quad (5)$$

where  $\eta$  is just a phase independent of  $k$  [26].

To apply the bosonization technique to this problem, one first shows that  $\mathcal{H}$  can be reduced exactly to an one-dimensional Hamiltonian. For that, one makes a projection on iso-energy surfaces in  $\vec{k}$  space; two  $\vec{k}$  are only retained by the Kondo effect and one can define the two following fields:

$$\Psi_{\pm,E} = \int d^3\vec{k} \delta(\epsilon(\vec{k}) - E) V(\pm\vec{k}) \Psi_{\vec{k}} \quad (6)$$

Hence, odd and even combinations of these two fields are defined:

$$\Psi_{e,E} = \frac{\Psi_{+,E} + \Psi_{-,E}}{N_e(E)}, \quad \Psi_{o,E} = \frac{\Psi_{+,E} - \Psi_{-,E}}{N_o(E)} \quad (7)$$

where

$$N_{e,o}(E) = \int d^3\vec{k} \delta(\epsilon(\vec{k}) - E) \cdot |V(\vec{k}) \pm V(-\vec{k})|^2 \quad (8)$$

to satisfy the anticommutation rules:  $\{\Psi_E, \Psi_E^\dagger\}_+ = \delta(E - E')$

Only these two fields appear in  $\mathcal{H}$  and we can rewrite:

$$\begin{aligned} H_o &= \int dE E [\Psi_{e,E}^\dagger \Psi_{e,E} + \Psi_{o,E}^\dagger \Psi_{o,E}], \\ H_k &= \int dE dE' [N_e(E) N_e(E') \Psi_{e,E}^\dagger \vec{\sigma} \Psi_{e,E'} + N_o(E) N_o(E') \Psi_{o,E}^\dagger \vec{\sigma} \Psi_{o,E'}] \cdot (\vec{S}_1 + \vec{S}_2) \\ &\quad + N_e(E) N_o(E') \cdot (\Psi_{e,E}^\dagger \vec{\sigma} \Psi_{o,E'} + \Psi_{o,E}^\dagger \vec{\sigma} \Psi_{e,E'}) \cdot (\vec{S}_1 - \vec{S}_2) \end{aligned} \quad (9)$$

Indeed, the one-dimensional problem has also a PH symmetry, deduced from the three-dimensional PH one. The problem of the particle-hole symmetry has been previously studied for the two-impurity  $s = \frac{1}{2}$  case [26,29], because in some special cases, one can develop some qualitative arguments for the variation with  $K$  of the phase shift of the conduction electrons and here, therefore, some insight on a possibility of a phase transition at a given  $K$  value.

The transformation of the fields  $\Psi_{e,E}$  and  $\Psi_{o,E}$  can be deduced from:

$$\Psi_{+,E} \longrightarrow \Psi_{+,-E}^\dagger, \quad \Psi_{-,E} \longrightarrow \Psi_{-,-E}^\dagger e^{i\eta} \quad (10)$$

obtained with the initial PH transformation.

In our case, we follow the method of Ref. [26] and we can select two particular values of  $\eta$ , i.e. ( $\eta=0$  and  $\eta=\pi$ ), which give arguments for two different physical behaviours.

For  $\eta=0$ , using the preceding PH one-dimensional transformation, one obtains:

$$N_e(-E) = N_e(E), \quad N_o(-E) = N_o(E), \quad \Psi_{e,E} \longrightarrow \Psi_{e,-E}^\dagger, \quad \Psi_{o,E} \longrightarrow \Psi_{o,-E}^\dagger \quad (11)$$

and for  $\eta = \pi$ , it results:

$$N_e(-E) = N_o(E), \quad \Psi_{e,E} \longrightarrow \Psi_{o,-E}^\dagger, \quad \Psi_{o,E} \longrightarrow \Psi_{e,-E}^\dagger \quad (12)$$

The case  $\eta = \pi$  is of particular interest. According to Ref. [26], the phase shifts  $\delta_e$  and  $\delta_o$  for the two fields given by (7) can take arbitrary values with the easily satisfied condition  $\delta_e = -\delta_o$ . Using the PH symmetry, it results only that a transition is not necessary in this case. The case  $\eta = 0$ , imposes  $\delta_e = \delta_o = 0$  or  $\delta_e = \delta_o = \frac{\pi}{2}$  and consequently a transition in the phase diagram. Finally, no universal behaviour can be predicted with a simple phase shift analysis.

Thus, we continue the calculation and write  $H_k$  given by (9) in a more suitable form, around  $E=0$ :

$$\begin{aligned} H_k = & \frac{1}{2} \int dE dE' J_+ (\Psi_{1,E}^\dagger \vec{\sigma} \Psi_{1,E'} + \Psi_{2,E}^\dagger \vec{\sigma} \Psi_{2,E'}) \cdot (\vec{S}_1 + \vec{S}_2) \\ & + J_m (\Psi_{1,E}^\dagger \vec{\sigma} \Psi_{1,E'} - \Psi_{2,E}^\dagger \vec{\sigma} \Psi_{2,E'}) \cdot (\vec{S}_1 - \vec{S}_2) \\ & + J_- (\Psi_{1,E}^\dagger \vec{\sigma} \Psi_{2,E'} + \Psi_{2,E}^\dagger \vec{\sigma} \Psi_{1,E'}) \cdot (\vec{S}_1 + \vec{S}_2) \end{aligned} \quad (13)$$

with the orthonormal basis:

$$\Psi_{1,2} = \frac{(\Psi_e \pm \Psi_o)}{\sqrt{2}} \quad (14)$$

and the couplings:



$$J_{\pm} = \frac{(J_e \pm J_o)}{\sqrt{2}}, \quad J_e = 2N_e(0)^2, \quad J_o = 2N_o(0)^2, \quad J_m = 2N_o(0)N_e(0) \quad (15)$$

When the asymmetry between the odd and even channels is not relevant, as for example in the case  $\eta = \pi$ , we get the following simplification:

$$N_e(0) = N_o(0), \quad J_m = J_+, \quad J_- = 0 \quad (16)$$

which will be used in the following.

We can notice that, whatever the maintained particle-hole symmetry is, the charges of the 1 and 2 species of fermions are separately conserved and we have two commuting sets of isospin generators; in fact, there is an exact  $O(4) = SU(2)_I * SU(2)_S$  symmetry on each channel:

$$\begin{aligned} I_1^z &= \frac{1}{2} \int dE \Psi_{1,E}^{\dagger\alpha} \Psi_{\alpha 1,E} \\ I_1^- &= \int dE \Psi_{\uparrow 1,E} \Psi_{\downarrow 1,-E} \end{aligned} \quad (17)$$

similarly for  $\vec{I}_2$ .

We just analyze the situation with an abelian symmetry (for the charge and spin degrees of freedom) and consequently, we have to break **explicitly** the  $O(4)$  one. We expect that the low-energy physics remains the same because a representation of the  $SU(2)$ ,  $k=1$  level algebra, with a central charge  $c=1$  can be satisfied by a representation of free bosons.

If now we try to calculate the preceeding values by taking the particular choice  $\epsilon(\vec{k}) = v_F(k - k_F)$  and by making the integration in the Eq.(6), we obtain:

$$N_{e,o}(k) = V_o \sqrt{1 \pm \frac{\sin(kR)}{kR}} \quad (18)$$

From the equalities (15), the couplings,  $J_m$ ,  $J_+$ ,  $J_-$  can be now easily evaluated:

$$J_+ = \pi \rho_F V_o^2, \quad J_- = \pi \rho_F V_o^2 * \frac{\sin(k_F R)}{k_F R}, \quad J_m = \pi \rho_F V_o^2 \sqrt{1 - \left(\frac{\sin(k_F R)}{k_F R}\right)^2} \quad (19)$$

where  $\rho_F$  is the density of states of the conduction electrons per spin at the Fermi level.

Thus,  $J_- = 0$  is equivalent to the equality  $k_F R = n\pi$ , where  $n$  is an integer; at half-filling this

constraint is realized for  $k_F = \frac{\pi}{2c}$  and consequently for an even impurity distance  $R = 2nc$ . In these conditions, by using the eq. (3) we deduce that a conventional RKKY interaction could only exist in the case of a parameter  $K \neq 0$  (since  $2k_F R = 2n\pi$ ).

Now, we make some comments about the feasible physical interpretation of  $\eta$  of the Ref. [26]. Indeed, if we take the definition (4) of  $V(\vec{k})$  and the second relation (5), we immediately obtain:

$$\eta = \frac{\vec{k}_o \cdot \vec{R}}{2} \quad (20)$$

where  $\vec{k}_o = \vec{k}' - \vec{k}$  and not  $\eta = \vec{k}_o \cdot \vec{R}$  already mentionned by Affleck et al. in Ref. [26].

In this context, the two values of  $\eta$  correspond either to  $\vec{k}_o=0$  or to the nesting vector  $\vec{k}_o = (\frac{\pi}{c}, \frac{\pi}{c}, \frac{\pi}{c})$ . With the condition  $R=2nc$  and the Eq. (20), we find that  $\eta = \pi * n$ , which yields  $\eta=0$  or  $\eta = \pi$  depending on the parity of  $n$ . We see that there is no universal behaviour and we cannot use this physical argument to conclude on the possibility of a critical point, in contrast to Ref. [26]; furthermore in the following, we will check that there is no critical point or even no phase transition in our  $S=1$  case.

By Fourier transform, we immediately obtain  $\mathcal{H}$ , in terms of two one-dimensional electronic channels  $a$  and  $b$ :

$$\mathcal{H} = H_o + K \vec{S}_1 \vec{S}_2 + J_+ \cdot (\vec{S}_1 + \vec{S}_2) [a^\dagger \frac{\vec{\sigma}}{2} a + b^\dagger \frac{\vec{\sigma}}{2} b]_{x=0} + J_m \cdot (\vec{S}_1 - \vec{S}_2) [a^\dagger \frac{\vec{\sigma}}{2} a - b^\dagger \frac{\vec{\sigma}}{2} b]_{x=0} \quad (21)$$

with

$$a(x) = \int dk e^{ikx} \Psi_1(k), \quad b(x) = \int dk e^{ikx} \Psi_2(k) \quad (22)$$

and

$$J_m = J_+ = J = \pi \rho_F V_o^2, \quad H_o = (iv_F) \sum_\sigma \int_{-\infty}^{+\infty} dx (a_\sigma^\dagger(x) \partial_x a_\sigma(x) + b_\sigma^\dagger(x) \partial_x b_\sigma(x)) \quad (23)$$

Within this model with  $J_m = J_+$ , no indirect magnetic interaction, i.e. via the conduction band, is generated up to the second order in perturbation between two half-spins, respectively

of  $S_1$  and  $S_2$ . Hence, we can assume that the Heisenberg interaction  $K\vec{S}_1\vec{S}_2$  takes into account both the indirect RKKY interaction and the direct one between the two S=1 spins.

## B. The bosonization

Thus, in the following, we start from the form (21) of the Hamiltonian for two S=1 spins and, as previously done for the case of two  $s = \frac{1}{2}$  spins, we use the bosonization technique by taking the standard 1-dimensional relations between Bose and Fermi fields [30]:

$$\Psi(x) = \frac{1}{2\pi c} \exp i\Phi_\psi(x) \quad (24)$$

$$\psi = a_\uparrow, a_\downarrow, b_\uparrow, b_\downarrow$$

$$\Phi_\psi = -\sqrt{\pi}(\phi_\psi + \int_{-\infty}^x \pi_\psi(x')dx')$$

$\phi_\psi$  and  $\pi_\psi$  are respectively a bosonic field and its conjugate field; as usual, the lattice spacing  $c$  is taking as tending to zero. In  $\mathcal{H}$ , the two electronic channels  $a$  and  $b$  are independent, then there is no need to introduce any phase factor in the  $\Psi$  field definition to take care of the anticommutation rules between the two different "species" of fermions [31]. Then, we just redefine four new bosonic fields that we call respectively charge, spin, spin-channel and charge-channel fields, obtained from the preceding ones by a linear canonical transformation:

$$\Phi_c = \frac{1}{2}(\Phi_{c,a} + \Phi_{c,b}), \quad \Phi_s = \frac{1}{2}(\Phi_{s,a} + \Phi_{s,b}), \quad (25)$$

$$\Phi_{sf} = \frac{1}{2}(\Phi_{s,a} - \Phi_{s,b}), \quad \Phi_{cc} = \frac{1}{2}(\Phi_{c,a} - \Phi_{c,b}) \quad (26)$$

where  $\Phi_{c,i}$  and  $\Phi_{s,i}$  are the charge and the spin fields for the  $i=a, b$  channels. The degrees of charge are frozen, thus it is clear that  $\Phi_c$  and  $\Phi_{cc}$  are not coupled to the impurities and we can omit them.

Thus, it comes:

$$H_o = \frac{v_F}{2} \sum_{\lambda=s, sf} \int_{-\infty}^{+\infty} dx \{ \Pi_\lambda^2 + [\partial_x \phi_\lambda]^2 \} \quad (27)$$

$$\begin{aligned}
H_k = & \frac{J_{z,+}}{\pi}(S_1^z + S_2^z)\nabla\Phi_s(0) + \frac{J_{m,z}}{\pi}(S_1^z - S_2^z)\nabla\Phi_{sf}(0) \\
& + \frac{J}{\pi c}\cos\Phi_s f(0)\{\cos\Phi_s(0)(S_1^x + S_2^x) - \sin\Phi_s(0)(S_1^y + S_2^y)\} \\
& - \frac{J}{\pi c}\sin\Phi_s f(0)\{\sin\Phi_s(0)(S_1^x - S_2^x) + \cos\Phi_s(0)(S_1^y - S_2^y)\}
\end{aligned}$$

The Kondo couplings  $J_{z,+}$  and  $J_{m,z}$  can take different values in the (x,y) plane and along the z axis. We can then perform a rotation along the quantization axis to eliminate  $\Phi_s$ . This type of procedure which originated from Ref. [32] was, for instance, used in the study of the two-channel one-impurity Kondo problem [33–35]. This can be achieved by considering the canonical transformation, in the unit sphere,  $U = \exp(-i(S_1^z + S_2^z))\Phi_s(0)$ . The effect of the rotation is to replace the trigonometric functions of  $\Phi_s(0)$  in Eq. (27) by their values at zero argument.

We obtain therefore:

$$\begin{aligned}
H_k = & \frac{J_{z,+} - \rho_F^{-1}}{\pi}(S_1^z + S_2^z)\nabla\Phi_s(0) + \frac{J_{m,z}}{\pi}(S_1^z - S_2^z)\nabla\Phi_{sf}(0) \\
& + \frac{J}{\pi c}\{\cos\Phi_s f(0)(S_1^x + S_2^x) - \sin\Phi_s f(0)(S_1^y - S_2^y)\}
\end{aligned} \tag{28}$$

where  $\rho_F$  is the density of states at the Fermi level for the conduction electrons  $\Psi_s = e^{i\Phi_s(x)}$ . The  $H_i$  coupling is not really affected by the transformation:

$$H_i = K_z S_1^z S_2^z + K S_1^+ S_2^- . \tag{29}$$

The canonical transformation also generates a positive constant term proportional to  $(S_1^z + S_2^z)^2 = 2S_1^z S_2^z + \frac{1}{2}$ , which can be reabsorbed in the  $K_z$  term and a negative coupling  $J_{z,+}(S_1^z + S_2^z)^2$  [31].

Now, we have to fix the  $J_{z,+}$  and  $J_{m,z}$  couplings. The  $J_{z,+}$  one can be integrated out using a path integral formalism; it only renormalizes the RKKY interaction [31]. This can be realized directly in tuning  $K$  and  $K_z$ . Thus, in the following, we set  $J_{z,+} = \rho_F^{-1}$ . When  $K=0$  we have chosen the particular case where the charges of the a and b electronic channels

are separately conserved and for that we could not keep  $J_{m,z}$  as a tunable parameter; from the Hamiltonian (28), in using Eqs. (25), (26) we have to take  $J_{m,z} \rightarrow 0$ . By analogy with the Toulouse limit, first discovered in the ordinary Kondo problem [36], we expect that this model is solvable at the particular point:  $J_{z,+} = \rho_F^{-1}$  and  $J_{m,z}=0$ . Now, we look at the Kondo problem in the transverse direction as keeping  $J = J_m$ , but allow  $J_{m,z} \neq J_{z,+} = \rho_F^{-1}$ :

$$\mathcal{H} = H_o + \frac{J}{2\pi c} \{S_1^+ e^{i\Phi_{sf}(0)} + e^{i\Phi_{sf}(0)} S_2^-\} + H_i \quad (30)$$

### III. THE STUDY OF THE TWO-IMPURITY S=1 UNDERSCREENED KONDO PROBLEM

In the preceding section, we have presented the general formalism appropriate for the two-impurity Kondo problem and we have finally obtained the form (30) of the total Hamiltonian, which is valid for any value of the spin. Then, we study the specific case of two S=1 spins and for that we decompose the two S=1 spins,  $S_1$  and  $S_2$ , into two 1/2-spins, as follow:

$$\vec{S}_1 = \vec{\tau}_1 + \vec{\tau}_2 \quad (31)$$

$$\vec{S}_2 = \vec{\tau}_3 + \vec{\tau}_4$$

where,  $\{\vec{\tau}_i\}_{(1,2,3,4)}$  are half SU(2) spins, which satisfy:

$$\{\tau_i^+, \tau_j^-\}_- = 0 \quad (32)$$

$$\{\tau_i^+, \tau_i^-\}_+ = 1, \quad \text{for } i=1, 2, 3, 4 \text{ and } j=1, 2, 3, 4$$

Indeed, we could not enlarge the total Hilbert space of the problem; so we add the constraint that  $\vec{\tau}_1, \vec{\tau}_2$  and  $\vec{\tau}_3, \vec{\tau}_4$  are strongly ferromagnetically coupled through an infinite  $-M_z$  ( $M_z \downarrow 0$ ) coupling. Then, we will solve the Hamiltonian given by (30) with the transformations (31). To do it, we refermionize the Hamiltonian (30) with spinless fermions by use of the Jordan-Wigner transformation and then we use a mean-field approximation which keeps terms containing at most four operators.

## A. Refermionization

In the following, we use the conduction electron operator:

$$\Psi = \frac{1}{2\pi c} \exp(i\Phi_{sf}(0)) \quad (33)$$

To refermionize this problem of four sets of Pauli matrices, we use the Jordan-Wigner transformation [37] for four spins:

$$\begin{aligned} \tau_1^+ &= d_1^\dagger \\ \tau_2^+ &= d_2^\dagger \cdot \exp(i\pi n_1) \\ \tau_3^+ &= d_3^\dagger \cdot \exp(i\pi(n_1 + n_2)) \\ \tau_4^+ &= d_4^\dagger \cdot \exp(i\pi(n_1 + n_2 + n_3)) \\ \tau_i^z &= d_i^\dagger d_i - \frac{1}{2}, \quad \text{with } n_i = 0, 1 \text{ for } i=1, 2, 3, 4 \end{aligned} \quad (34)$$

Then, we develop  $\mathcal{H}$  in power of  $(n_i \cdot n_j)$ , with  $i=1, 2, 3, 4$  and  $j=1, 2, 3, 4$ , in using the shrewd identity:

$$\exp(i\pi n) = 1 - 2n \quad \text{for } n=0 \text{ or } 1 \quad (35)$$

Thus, applying the different transformations (33),(34),(35) on the reduced Hamiltonian (30) yields many terms containing products of operators  $\Psi$  and  $d_i$ ; in particular, we get several terms containing more than 4 spinless fermion operators, such as for example  $d_1^\dagger d_4 n_2 n_3$  (obtained from  $H_i$ ) or  $\Psi d_4 n_2 n_3$  (obtained from  $H_k$ ). In order to solve the problem we use here a special mean-field approximation, which consists in firstly keeping only terms containing at most four operators and then making averages on terms with two operators. In fact, as we will see in the following, we will use a mean-field approximation which linearizes the terms in the Hamiltonian and keeps only terms which are bilinear in the spinless fermion operator  $d$ . This approximation had already been used in Ref. [28] for the  $s = \frac{1}{2}$  two-impurity problem. We have to remember the two following points induced by the transform (31):  $\tau_1, \tau_2$  interact with the same conduction electron and  $\tau_3, \tau_4$  with another one, while  $\langle \vec{\tau}_1 \vec{\tau}_3 \rangle = \langle \vec{\tau}_2 \vec{\tau}_4 \rangle$  and  $\langle \vec{\tau}_1 \vec{\tau}_4 \rangle = \langle \vec{\tau}_2 \vec{\tau}_3 \rangle$ , but not necessarily  $\langle \vec{\tau}_1 \vec{\tau}_3 \rangle = \langle \vec{\tau}_1 \vec{\tau}_4 \rangle$ .

Then, using the preceding approximations, the total Hamiltonian can be written in terms of fermionic spinless operators:

$$\begin{aligned}
\mathcal{H} &= H_k + H_{int} + H_o, \text{ with} \\
H_o &= iv_F \int_{-\infty}^{+\infty} dx \Psi^\dagger(x) \partial_x \Psi(x) \\
H_k &= H_a + H_+ \\
H_{int} &= H_{i,\parallel} + H_{i,\perp} + H_{ferro}
\end{aligned} \tag{36}$$

$H_a$  describes the Kondo problem when the two  $S=1$  spins are not coupled,  $H_+$  brings a new Kondo contribution coming from the K interaction and  $H_{ferro}$  is added here to take into account the decomposition of the  $S=1$  spins (with the assumption  $M_z \rightarrow \infty$ ):

$$\begin{aligned}
H_a &= J\Psi(d_1^\dagger + d_2^\dagger) - J\Psi d_1^\dagger n_2 - J\Psi d_2^\dagger n_1 \\
&\quad - J\Psi(d_3 + d_4) + J\Psi d_3 n_4 + J\Psi d_4 n_3 \\
H_+ &= J\Psi(d_3 + d_4)\{n_1 + n_2\} - J\Psi(d_1^\dagger + d_2^\dagger)\{n_3 + n_4\} \\
H_{i,\perp} &= \frac{K}{2}\{d_1^\dagger d_3(1 - 2n_2 - 2n_4) + d_1^\dagger d_4(1 - 2n_2 - 2n_3) \\
&\quad + d_2^\dagger d_3(1 - 2n_4 - 2n_1) + d_2^\dagger d_4(1 - 2n_3 - 2n_1) + hc\} \\
H_{i,\parallel} &= K_z\{d_1^\dagger d_1 + d_2^\dagger d_2 - 1\}\{d_3^\dagger d_3 + d_4^\dagger d_4 - 1\} \\
H_{ferro} &= -M_z(d_1^\dagger d_1 - \frac{1}{2})(d_2^\dagger d_2 - \frac{1}{2}) - M_z(d_3^\dagger d_3 - \frac{1}{2})(d_4^\dagger d_4 - \frac{1}{2})
\end{aligned} \tag{37}$$

## B. The case $K = 0$

As previously explained, our presently studied case  $J_m = J_+$  corresponds to a situation where the indirect and direct interactions between  $\vec{S}_1$  and  $\vec{S}_2$  are yielded only by the additive term  $K\vec{S}_1\vec{S}_2$ . Thus, the case  $K=0$  corresponds to two initial  $S=1$  spins which are decoupled from each other and the physics of this problem is similar to that of the one  $S=1$ ,  $n=1$  Kondo impurity. It results that the term  $H_+$  of the Hamiltonian must have no effect and that  $\mathcal{H}$  can be divided into two independent underscreened Kondo problems:

$$H_{H_i=0} = H_{1,2} + H_{3,4} + H_o \quad (38)$$

with

$$\begin{aligned} H_{1,2} = & J\Psi(d_1^\dagger + d_2^\dagger) - J\Psi d_1^\dagger n_2 - J\Psi d_2^\dagger n_1 \\ & - M_z(d_1^\dagger d_1 - \frac{1}{2})(d_2^\dagger d_2 - \frac{1}{2}) \end{aligned} \quad (39)$$

and

$$\begin{aligned} H_{3,4} = & -J\Psi(d_3 + d_4) + J\Psi d_3 n_4 + J\Psi d_4 n_3 \\ & - M_z(d_3^\dagger d_3 - \frac{1}{2})(d_4^\dagger d_4 - \frac{1}{2}) \end{aligned} \quad (40)$$

We study this case  $K=0$ , in order to fix the theoretical notations for the following studies.

Then, in our present case, we can easily derive the following equalities for the average values:

$$\begin{aligned} \langle d_1^\dagger d_2 \rangle &= \langle d_3^\dagger d_4 \rangle, & \langle d_1^\dagger d_2^\dagger \rangle &= \langle d_3^\dagger d_4^\dagger \rangle \\ \langle \Psi d_1^\dagger \rangle &= -\langle \Psi d_3 \rangle, & \langle \Psi d_2^\dagger \rangle &= -\langle \Psi d_4 \rangle \\ \langle \Psi d_1 \rangle &= -\langle \Psi d_3^\dagger \rangle, & \langle \Psi d_4 \rangle &= -\langle \Psi d_2 \rangle \end{aligned} \quad (41)$$

We describe here the  $S=1$  spins by adding two  $s = \frac{1}{2}$  spins ferromagnetically aligned, according to the last terms of (39) and (40) with  $M_z$  tending to  $+\infty$ . As in ref. [28], the last term of (39) can be decoupled in the mean-field approximation into:

$$\frac{-M_z}{2} \left\{ \langle n_2 - \frac{1}{2} \rangle \langle n_1 - \frac{1}{2} \rangle + \langle n_1 - \frac{1}{2} \rangle \langle n_2 - \frac{1}{2} \rangle \right\} + \frac{M_z}{2} \langle d_1^\dagger d_2 \rangle \{ d_1^\dagger d_2 + d_2^\dagger d_1 \} - \frac{M_z}{2} \langle d_1^\dagger d_2^\dagger \rangle \{ d_1^\dagger d_2^\dagger + d_2 d_1 \}$$

The first term does not contribute due to the effective particle-hole (PH) symmetry. However, our present case of two  $S=1$  spins is clearly original and we have to examine the solution occuring for a very strong ferromagnetic coupling  $M_z \rightarrow +\infty$ . If we consider the energy of the system, it is necessary to stabilize it to take both  $\langle d_1^\dagger d_2 \rangle$  tending to 0 for  $M_z \rightarrow +\infty$  and  $\langle d_1^\dagger d_2^\dagger \rangle$  tending to its maximum value, which must be equal to  $\langle d_1^\dagger d_2^\dagger \rangle = 1$ .



It results that the first three terms of  $H_{1,2}$  given by (39), treated within the preceding mean field approximation, become equal to  $J\Psi[d_1^\dagger + d_2^\dagger + (d_1 - d_2)\langle d_1^\dagger d_2^\dagger \rangle]$  and it results a new important contribution  $J\Psi(d_1 - d_2)$  for  $\langle d_1^\dagger d_2^\dagger \rangle = 1$ , in addition to the first term  $J\Psi(d_1^\dagger + d_2^\dagger)$ .

For the physical limit  $M_z \rightarrow +\infty$  corresponding to a S=1 spin, we can rewrite  $H_{1,2}$  in the following form:

$$H_{1,2} = J\Psi(d_1^\dagger + d_2^\dagger + d_1 - d_2) + h(d_1^\dagger d_2^\dagger + d_2 d_1) + H_o \quad (42)$$

where  $h$  is determined by the following self-consistent equations:

$$h = -\frac{M_z}{2} + J\langle \Psi d_1 \rangle \rightarrow -\infty \quad (43)$$

and

$$\langle \Psi d_1^\dagger \rangle = \langle \Psi d_2^\dagger \rangle = \langle \Psi d_1 \rangle = -\langle \Psi d_2 \rangle \quad (44)$$

We can deduce that, due to the strong pairing mechanism between  $d_1$  and  $d_2$ , only one degree of freedom is coupled to the conduction band: half a degree of freedom for the 1<sup>st</sup> spinless fermion  $\frac{(d_1^\dagger + d_1)}{2}$  and half a degree of freedom for the 2<sup>nd</sup> spinless fermion  $\frac{(d_2^\dagger - d_2)}{2}$ .

Then, to make the Kondo problem more explicit, we redefine two new spinless fermions  $d$  and  $D$  by the simple linear transformation:

$$d^\dagger = (a_1 + ib_2), \quad d = (a_1 - ib_2), \quad D^\dagger = (a_2 + ib_1), \quad D = (a_2 - ib_1) \quad (45)$$

with

$$a_1 = \frac{(d_1^\dagger + d_1)}{2}, \quad a_2 = \frac{(d_2^\dagger + d_2)}{2}, \quad ib_1 = \frac{(d_1^\dagger - d_1)}{2}, \quad ib_2 = \frac{(d_2^\dagger - d_2)}{2} \quad (46)$$

One can easily check that the different operators satisfy the good anticommutation rules. Only the  $d$  fermion is resonant and is coupled to the conduction band through a coupling  $J^* = 2J$ . Consequently, the  $d$  and  $D$  fermions are not coupled anymore, the  $h$  coupling just shifts the resonant  $d$ -level at the Fermi energy  $E_d = E_F = -h$  and makes the  $D$ -level lying at the energy  $E_D = h$ . As usual, we redefine the Fermi energy  $E_F = 0$  and consequently  $E_D = 2 * h$ . Thus, the Hamiltonian  $H_{1,2}$  can be written as:

$$H_{1,2} = J^* \Psi d^\dagger + E_D \cdot D^\dagger D \quad (47)$$

Then, for the fermions  $d_3$  and  $d_4$ , we propose the same relations:

$$e^\dagger = (a_3 + ib_4), \quad e = (a_3 - ib_4), \quad E^\dagger = (a_4 + ib_3), \quad E = (a_4 - ib_3) \quad (48)$$

with

$$a_3 = \frac{(d_3^\dagger + d_3)}{2}, \quad a_4 = \frac{(d_4^\dagger + d_4)}{2}, \quad ib_3 = \frac{(d_3^\dagger - d_3)}{2}, \quad ib_4 = \frac{(d_4^\dagger - d_4)}{2} \quad (49)$$

Finally, for  $K = 0$ , the total Hamiltonian  $\mathcal{H}$ , can be written as two usual "not-coupled" resonant levels [38]:

$$\mathcal{H}_{K=0} = J^* \Psi d^\dagger + J^* \Psi^\dagger e^\dagger + H_o^* \quad (50)$$

with:

$$H_o^* = H_o + E_D \cdot (D^\dagger D + E^\dagger E) \quad (51)$$

It is well-known that this model is isomorphic to the usual Kondo effect at a certain particular point namely the Toulouse limit [36]:

$$\begin{aligned} \mathcal{H}_{K=0} = & J^* s_1^\dagger (a_\downarrow^\dagger a_\uparrow) + J^* s_3^\dagger (b_\downarrow^\dagger b_\uparrow) \\ & + G_z s_1^z (a_\uparrow^\dagger a_\uparrow - a_\downarrow^\dagger a_\downarrow) + G_z s_3^z (b_\uparrow^\dagger b_\uparrow - b_\downarrow^\dagger b_\downarrow) + H_o \end{aligned} \quad (52)$$

with

$$G_z = 0 = J_z^* - \frac{2}{\rho_F} \quad (53)$$

where

$$\vec{s}_1 \quad \text{and} \quad \vec{s}_2 \in \vec{S}_1 \quad \text{with} \quad |\vec{s}_1| = |\vec{s}_2| = \frac{1}{2} \quad (54)$$

and:

$$\vec{s}_3 \quad \text{and} \quad \vec{s}_4 \in \vec{S}_2 \quad \text{with} \quad |\vec{s}_3| = |\vec{s}_4| = \frac{1}{2} \quad (55)$$

The model (52) describes two similar Kondo effects acting on different sites, each characterized by the energy scale that we call  $T_k$ . The strong fixed point of this problem ( $J^*, J_z^* \rightarrow +\infty$ ) is stable and corresponds to the well-known Fermi-liquid behaviour: the channel a interacts with the half  $s_1$  spin of  $S_1$  and the channel b interacts with the half  $s_3$  spin of  $S_2$ . It remains on each site a  $s = \frac{1}{2}$  "not screened" local moment:  $s_2 \in S_1 = 1$ ,  $s_4 \in S_2 = 1$ . It is remarkable to notice that these residual moments are totally decoupled from the conduction band and from  $s_1$  and  $s_3$  respectively. Consequently, the conduction electrons are submitted to a phase shift  $\delta = \frac{\pi}{2}$  induced by the infinite local Kondo coupling. In fact, we have solved the case  $K=0$ , at a particular solvable limit, where the Kondo coupling is not infinite and we could expect that the half-spins  $s_2$  and  $s_4$  are not exactly totally decoupled from the conduction band; anyway, the physics is not changed.

The mean-field treatment appears quite efficient to treat the Kondo problem without any interaction  $K=0$  between the two concerned  $S=1$  Kondo impurities and we will discuss in the following the non zero  $K$  cases.

### C. The ferromagnetic coupling ( $K \neq 0$ )

Now we look briefly at a ferromagnetic coupling  $K \vec{S}_1 \vec{S}_2$ , with  $K < 0$ . As shown before, an RKKY interaction is not expected in this case and  $K$  concerns (simply) a direct exchange between the two  $S=1$  spins, according to the discussion after eq. (19). We just develop qualitative arguments concerning the phase shift  $\delta$  of the conduction electrons induced by the local Kondo effect. Indeed, if we consider that the system starts, from  $K=0$ , with an infinite Kondo coupling ( $\delta = \frac{\pi}{2}$ ) and finally goes towards  $K \rightarrow -\infty$  with the same stable Kondo situation ( $\delta = \frac{\pi}{2}$ ), we do not expect (in the area  $K < 0$ ) any particular critical point

where the phase shift of the conduction electrons would not be defined. We even expect a Kondo effect of magnitude of  $T_k$  for all  $K \neq 0$ .

In fact, our mean-field treatment is not well appropriate for the direct ferromagnetic K interaction, but our preceding qualitative arguments are sufficient to conclude that there is no critical point for  $K \neq 0$ , as in the two  $s = \frac{1}{2}$  impurity case.

#### D. The antiferromagnetic coupling ( $K \neq 0$ ).

The most interesting case corresponds to an antiferromagnetic coupling ( $K \neq 0$ ), because in this case it is important to study the absence or existence of a phase transition, even a critical point as a function of  $K$ , by analogy with the two  $s = \frac{1}{2}$  impurity case where a sharp phase transition occurs for  $K$  of order  $2T_k$ .

However, we will use the mean-field approximation as in the previous  $K=0$  case and we treat the case of moderate  $K$  values, where we can apply only a small perturbation from the  $K=0$  results; finally, it is sufficient since if a critical point exists, it is certainly not so far from the particular point  $K=0$ .

Thus, we keep here  $\langle d_1^\dagger d_2^\dagger \rangle = \langle d_3^\dagger d_4^\dagger \rangle = 1$  as previously shown and we consider all the other averages of two operators as small quantities.

The mean-field approach gives, therefore:

$$H_{i,\perp} = \frac{K}{2} \{ (d_1^\dagger + d_2^\dagger)(d_3 + d_4) + 4(d_1^\dagger d_4^\dagger + d_3^\dagger d_2^\dagger) + hc \} \quad (56)$$

$$H_{i,\parallel} = \frac{K_z}{2} \{ \langle d_1^\dagger d_4^\dagger \rangle (d_1^\dagger d_4^\dagger + d_3^\dagger d_2^\dagger) - \sum_{\alpha=1,2, \beta=3,4} \langle d_\alpha^\dagger d_\beta \rangle d_\alpha^\dagger d_\beta + hc \} \quad (57)$$

We can notice that it is consistent with the mean-field equations to consider  $\langle d_\alpha^\dagger d_\beta \rangle_{(\alpha=1,2, \beta=3,4)}$  and  $\langle d_\alpha^\dagger d_\beta^\dagger \rangle_{(\alpha=1,2, \beta=3,4)}$  as real. Using the Eqs. [(56),(57)], we deduce also that, due to the nonzero  $K$  coupling, the antiferromagnetic correlations favorize both the pairing mechanism (particle1, particle4) or (particle2, particle3) and the binding mechanism of a particle  $\alpha$  ( $\alpha = 1, 2$ ) with a hole  $\beta$  ( $\beta = 3, 4$ ); hence, in contrast to the case of two

$s = \frac{1}{2}$  Kondo impurities [28], there is no competition anymore between these two kinds of processes but either a good coexistence; we can add that it could be an important argument for the non existence of a phase transition in the area  $K \sim T_k$ .

Then, we assume that  $H_+$  can be treated as a perturbation of  $H_a$ , by considering that the mean-field symmetries of equations (44) are preserved. By use of all the previous arguments, the couplings  $K$  and  $K_z$  renormalize the operators  $\langle d_\alpha^\dagger d_\beta \rangle_{(\alpha=1,2, \beta=3,4)}$  at the same negative value,  $\langle d_1^\dagger d_4^\dagger \rangle = \langle d_3^\dagger d_2^\dagger \rangle$  at a positive constant value, maintain  $\langle d_1^\dagger d_3^\dagger \rangle$  and  $\langle d_2^\dagger d_4^\dagger \rangle$  at zero and make  $H_+$  relevant.  $\mathcal{H}$  becomes finally equal to:

$$\begin{aligned} \mathcal{H} = & \mathcal{H}_{K=0} + J_1 \Psi(d_3^\dagger + d_4^\dagger - d_1 - d_2) + J_2 \Psi(d_2^\dagger - d_1^\dagger + d_3 - d_4) \\ & + \{h_1[(d_1^\dagger + d_2^\dagger)(d_3 + d_4) + h.c.] + h_2[(d_1^\dagger d_4^\dagger + d_3^\dagger d_2^\dagger) + h.c.]\} \end{aligned} \quad (58)$$

with the following self-consistent equations:

$$\begin{aligned} J_1 &= 2J\langle d_1^\dagger d_3 \rangle, & J_2 &= J\langle d_1^\dagger d_4^\dagger \rangle \\ h_2 &= -2K + \frac{K_z}{2}\langle d_1^\dagger d_4^\dagger \rangle, & h_1 &= \frac{K}{2} - \frac{K_z}{2}\langle d_1^\dagger d_3 \rangle \end{aligned} \quad (59)$$

For an antiferromagnetic coupling, i.e. for positive  $K$  and  $K_z$  values, one can easily show that  $J_2$  and  $h_1$  are positive, while  $J_1$  and  $h_2$  are negative; we have also  $h_2 \sim -4h_1$  for small values of  $\langle d_1^\dagger d_4^\dagger \rangle$  and  $\langle d_1^\dagger d_3 \rangle$  corresponding to very small values of  $K$ . In principle, we would have to solve within the mean-field approximation the system of self-consistent equations based on the Hamiltonian (58) and the relations (59). However, the system is quite tricky to solve and we can have already a good insight of the physics in looking simply at the solutions obtained within the subspace of operators  $d$  and  $D$  (or  $e$  and  $E$ ) introduced for  $K=0$ .

Then, we use the equations (45),(46),(48) and(49) in order to transform the total Hamiltonian, which becomes:

$$\mathcal{H} = H_o^* + H_{res} + H_{coupling} \quad (60)$$

with

$$H_{coupling} = (h_1 + h_2)(E^\dagger D + D^\dagger E) + (h_1 - h_2)(e^\dagger d + d^\dagger e) + h_1(E^\dagger d + e^\dagger D + hc) \quad (61)$$

$$H_{res} = J^* \Psi(d^\dagger - e) + J_o^*(D^+ - E)\Psi^\dagger \quad (62)$$

and

$$J_o^* = J_2 - J_1 \quad (63)$$

We have not considered in the equation (62) the small contribution  $(J_1 + J_2)\Psi^\dagger d^\dagger$ , because the  $d$  operator is strongly resonant with the large  $J^*$  coupling and  $(J_1 + J_2)$  is very small; so, this very small coupling in  $(J_1 + J_2)$  is negligible with respect to the very large one in  $J^*$  and does not change the physics of the problem .

In spite of the peculiar mean-field treatment, the solutions given by the above equations yield a good insight on the physics of the two S=1 impurity case.  $J_o^*$ , which is irrelevant for K=0, becomes really relevant for an antiferromagnetic coupling.

The crucial point concerns here the non existence of a critical point or any kind of phase transition as a function of the K parameter, since there is no Green function divergent when  $\omega \rightarrow 0$  for the considered set of parameters. In fact, we have obtained for the two main Green functions (the others vary as  $K^2$ ):

$$G_{dd^\dagger}(\omega) = \frac{-i(\omega \pm \Gamma_k)\{\omega^2 \pm \Gamma_k\omega + h_1^2 + (h_1 - h_2)^2\}}{(\omega^2 \pm \Gamma_k\omega + h_1^2 + (h_1 - h_2)^2)^2 - 4h_1^2(h_1 - h_2)^2} \quad (64)$$

and

$$G_{DD^\dagger}(\omega) = \frac{-i(\omega \pm \Gamma_o^*)\{\omega^2 \pm \Gamma_o^*\omega + h_1^2 + (h_1 + h_2)^2\}}{(\omega^2 \pm \Gamma_o^*\omega + h_1^2 + (h_1 + h_2)^2)^2 - 4h_1^2(h_1 + h_2)^2} \quad (65)$$

where  $\omega = (2n+1)\pi/\beta$  is a fermionic Matsubara frequency  $\Gamma_k = \rho J^{*2}$  and  $\Gamma_o = \rho J_o^{*2} \ll \Gamma_k$  are respectively the widths of the  $d$  and  $D$  (respectively the  $e$  and  $E$ ) impurity levels,  $\Gamma_o^* = \Gamma_o + iE_D$  and  $\Gamma_k$  is of order  $T_k$ . In Eqs. (64) and (65), the upper and lower sign corresponds respectively to the case of positive and negative  $\omega$ . Indeed, the different Green functions do not develop a pole at  $\omega = 0$ , whatever the values of  $\Gamma_k$  and  $\Gamma_o$  are and we do not expect any

critical point at low temperatures. Especially, we expect that the staggered susceptibility  $\chi_s$  does not diverge [28].

Simply, when  $K$  and  $K_z$  are small, we can neglect the terms in  $h_1^2$  and  $h_2^2$  and therefore, write the two (main) Green functions:

$$\begin{aligned} G_{dd^\dagger}(\omega) &= \frac{1}{i\omega \pm i\Gamma_k} = G_{ee^\dagger} \\ G_{DD^\dagger}(\omega) &= \frac{1}{i\omega \pm i\Gamma_o^*} = G_{EE^\dagger} \end{aligned} \tag{66}$$

The influence of  $K$  appears mainly through the magnitude  $\Gamma_o$ . So, when  $K$  is small, it appears two cohabiting species of quasiparticles: heavy quasiparticles with an electronic specific heat constant  $C/T = \Gamma_k^{-1}(K) = \chi$  and quasi-free electrons which lead to the main RKKY interaction between the non-screened half-spins, namely  $s_2$  and  $s_4$  (already introduced for  $K=0$ ) and generated by a small ferromagnetic Kondo coupling due to the Pauli principle. In fact, other marginal RKKY interactions also exist, which couple all the half-spins and which, especially guarantee exact physics in the strong  $K$ -coupling limit; however, they are not really relevant, for small values of  $K$  and can be forgotten.

Indeed, all these conclusions are done, at a particular solvable point and we can not be exactly sure that they remain true for any value of  $J$ ; nevertheless, we think that these results are physically correct and then, the fixed point of the coupling  $J$  has to decrease with  $K$ . Precisely, the dominant RKKY interaction (between  $s_2$  and  $s_4$ ) tends to suppress the critical point, obtained with the two  $s=1/2$  Kondo impurity-model and yields both a Kondo effect and magnetism, for small positive  $K$  values.

#### IV. CONCLUSION

In this paper, we have presented an explicit study of the problem of two  $S=1$  magnetic impurities interacting with a conduction band and coupled via an interimpurity coupling  $K\vec{S}_1.\vec{S}_2$ . There is no quantum critical point, even no phase transition in the phase diagram

and this last point is very important because it shows a behaviour completely different from that of the regular two screened  $s = \frac{1}{2}$  impurity Kondo model. In fact, a **smooth** cross-over separates a “one-underscreened-Kondo-impurity” like phase from an antiferromagnetic and non-Kondo phase. In particular, it leads that  $\delta = \arctan(J^*)$  and  $\frac{\partial}{\partial K}\langle\vec{S}_1\vec{S}_2\rangle$  vary continuously with  $K$ , for all the real values of this parameter.

We have obtained, for a positive and small  $K$  value, an asymmetric situation with a strong Kondo effect for the spins  $s_1$  and  $s_3$ , a weak Kondo effect for the spins  $s_2$  and  $s_4$  and finally a RKKY interaction between  $s_2$  and  $s_4$ . This can lead to a coexistence between a Kondo effect leading to strong spin fluctuations on one side and an indirect RKKY interaction. Finally, with only two spins, a true magnetic order and a really broken  $SU(2)$  spin symmetry could not occur but it is encouraging to yield, even in this particular case, a coexistence between a heavy-fermion character and (special) magnetism.

Thus, the case of a moderate and antiferromagnetic  $K$  coupling can account for the physics of Uranium compounds, such as  $UPt_3$ , where both a heavy-fermion behaviour and some kind of long-range magnetic order exist at low temperatures. In any underscreened Kondo lattice model, the presence of magnetism is expected but much remains to be understood concerning the magnetic length of the intersite antiferromagnetic fluctuations or more generally concerning the tiny magnetic moment which characterizes the magnetic character of  $UPt_3$ , as already noticed by Coleman et al. [39]. Finally, a more complete explanation of the properties of compounds such as  $UPt_3$ , based on a non-Abelian treatment of the underscreened Kondo lattice, is presently studied [40].

## ACKNOWLEDGMENTS

One of us (K.L.H.) would like to thank Thierry Giamarchi for interesting discussions and remarks.



## REFERENCES

- [1] K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
- [2] B. Coqblin and J.R. Schrieffer, Phys. Rev. **185**, 847 (1969).
- [3] S. Doniach, Physica B**91**, 231 (1977).
- [4] B. Coqblin, J. Arispe, J.R. Iglesias, C. Lacroix and Karyn Le Hur, to J. Phys. Soc. Japan, **65** (1996) Suppl B, pp. 64-77.
- [5] G. Aeppli, E. Bucher, C. Broholm, J.K. Kjems, J. Baumann and J. Hufnagl, Phys. Rev. Lett. **60**, 615 (1988).
- [6] G.R. Stewart, Z. Fisk, J.O. Willis and J.L. Smith, Phys. Rev. Lett. **52**, 679 (1984); L. Taillefer, K. Behnia, K. Hasselbach, J. Flouquet, S.M. Hayden and C. Vettier, J. Magn. Mater. **90-91**, 623 (1990).
- [7] G.E. Brodale, R.A. Fisher, N.E. Phillips, G.R. Stewart and A.L. Giorgi, Phys. Rev. Lett. **57**, 234 (1986).
- [8] J.O. Willis, J.D. Thomson, Z. Fisk, A. de Visser, J.J.M. Franse and A. Menovsky, Phys. Rev. B**31**, 1654 (1985).
- [9] S.M. Hayden, L. Taillefer, C. Vettier and J. Flouquet, Phys. Rev. B**46**, 8675 (1992).
- [10] A. de Visser, Manuscript submitted to the International Conference on Strongly Correlated Electron Systems (Zürich, 15-18 August 1996).
- [11] A. de Visser, Manuscript submitted to the International Conference on Strongly Correlated Electron Systems (Zürich, 15-18 August 1996).
- [12] H.R. Ott, H. Rudigier, Z. Fisk and J.L. Smith, Phys. Rev. Lett. **50**, 1595 (1983); L. Taillefer, J. Flouquet and G.G. Lonzarich, Physica B**169**, 257 (1991).
- [13] T.T. Palstra, A.A. Menovsky, J. van den Berg, A.J. Dirkmaat, P.H. Kes, G.J. Nieuwen-

- huys and M.A. Mydosh, Phys. Rev. Lett. **55**, 2727 (1985).
- [14] C. Geibel, S. Thies, D. Kaczorowski, A. Mehner, A. Grauel, B. Seidel, R. Hefrich, K. Petersen, C. D. Bredl and F. Steglich, Z. Phys. **83**, 305 (1991).
- [15] C. Geibel, C. Schank, S. Thies, H. Kitazawa, C.D. Bredl, A. Bohm, M. Rau, R. Caspary, R. Hefrich, U. Ahlheim, G. Weber and F. Steglich, Z. Phys. **84**, 1 (1991).
- [16] M. Kyogaku, Y. Kitaoka, K. Asayama, C. Geibel, C. Schank and F. Steglich, J. Phys. Soc. Japan **62**, 4016 (1993).
- [17] R.N. Kleiman, D.J. Bishop, H.R. Ott, Z. Fisk and J.L. Smith, Phys. Rev. Lett. **64**, 1975 (1990).
- [18] A. Krimmel, P. Fisher, B. Roessli, H. Maletta, C. Geibel, C. Schank, A. Granel, A. Loidl and F. Steglich, Z. Phys. **B46**, 161, (1992).
- [19] A. de Visser, J. Flouquet, J.J.M. Franse, P. Haen, K. Hasselbach, A. Lacerda and L. Taillefer, Physica B **171**, 190 (1991).
- [20] F. Steglich, P. Gegenwart, C. Geibel, R. Helfrich, P. Hellmann, M. Lang, A. Link, R. Modler, G. Sparn, N. Büttgen and A. Loidl, Physica B **223-224**, 1 (1996).
- [21] W.J.L. Buyers, Physica B **223-224**, 9 (1996).
- [22] P. Nozières and A. Blandin, J.Physique. (Paris) **41**, 193 (1980).
- [23] D.M. Cragg and P. Lloyd, J.Phys.C **12**, L215 (1979).
- [24] V.A. fateev and P.B. Wiegmann, Phys. Rev. Lett. **46** (1981) 356; A.M. Tsvelik, Z. Phys. **54B** (1983) 201; N. Andrei and C. Destri, Phys. Rev. Lett. **52**, 364 (1984).
- [25] I. Affleck, Nucl.Phys, **B336**, 517, (1990), I. Affleck and A.W.W. Ludwig, Nucl.Phys, **B352**, 849 (1991), I. Affleck and A.W.W. Ludwig, Nucl.Phys, **B360**, 641-696 (1991).
- [26] I. Affleck, A.W.W. Ludwig and B.A. Jones Phys. Rev. B **52**, 9528 (1995).

- [27] R.M. Fye and J.E. Hirsch, Phys. Rev. B**40**, 4780 (1989); R.M. Fye and J.E. Hirsch, Phys. Rev. Lett. **72**, 916 (1994).
- [28] C. Sire, C.M. Varma and H.R. Krishnamurthy, Phys. Rev. B**48**, 13833 (1993).
- [29] I. Affleck, A.W.W. Ludwig, H-B. Pang and D.L. Cox, Phys. Rev. B**45**, 7918 (1992).
- [30] See, e.g, V.J. Emery, *in Highly Conducting One-Dimensional Solids*, edited by J.T. Devreese, R.P. Evrard and V.E. Van.Doren,(Plenum,New York,1979), p.327; J. Solyom, Adv.Phys. **28**, 201 (1979);S. Sachdev and R. Shankar, Phys. Phys. Rev. B**38**, 826 (1988).
- [31] J. Gan Phys, Phys. Rev. B**51**, 8287 (1995).
- [32] J. Emery and A. Luther, Phys. Rev. B**9**, 215 (1974).
- [33] V.J. Emery and S. Kivelson, Phys. Rev. B**46**, 10812 (1992).
- [34] D. G. Clarke, T. Giamarchi and B. I. Shraiman, Phys. Rev. B**48**, 7070 (1993).
- [35] A.M. Sengupta and A. Georges, Phys. Rev. B**49**, 10020 (1994).
- [36] G. Toulouse, Phys. Rev. B**2**, 270 (1970).
- [37] P. Jordan and E. Wigner, Z Phys. B **47**, 631 (1928).
- [38] P. Nozières and C. De. Dominicis, Phys. Rev. **178**, 1097 (1969), G. Yuval and P.W. Anderson, Phys. Rev. B**1**,1522 (1970), M. Fabrizio, A.O. Gogolin, P. Nozieres, Phys. Rev. B**51**, 16088 (1995).
- [39] J. Gan, P. Coleman and N. Andrei, Phys. Rev. Lett. **68**, 3476 (1992).
- [40] Karyn Le Hur and B. Coqblin, to be published.